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## FAST TRACK COMMUNICATION

# Field modulation in bilayer graphene band structure

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Online at [stacks.iop.org/JPhysCM/21/102202](http://stacks.iop.org/JPhysCM/21/102202)**Abstract**

Using an external electric field, one can modulate the band gap of Bernal stacked bilayer graphene by breaking the  $A-\tilde{B}$  symmetry. We analyze strain effects on the bilayer graphene using the extended Hückel theory and find that reduced interlayer distance results in higher band gap modulation, as expected. Furthermore, above about 2.5 Å interlayer distance, the band gap is direct, follows a convex relation with the electric field and saturates to a value determined by the interlayer distance. However, below about 2.5 Å, the band gap is indirect, the trend becomes concave and a threshold electric field is observed, which also depends on the stacking distance.

(Some figures in this article are in colour only in the electronic version)

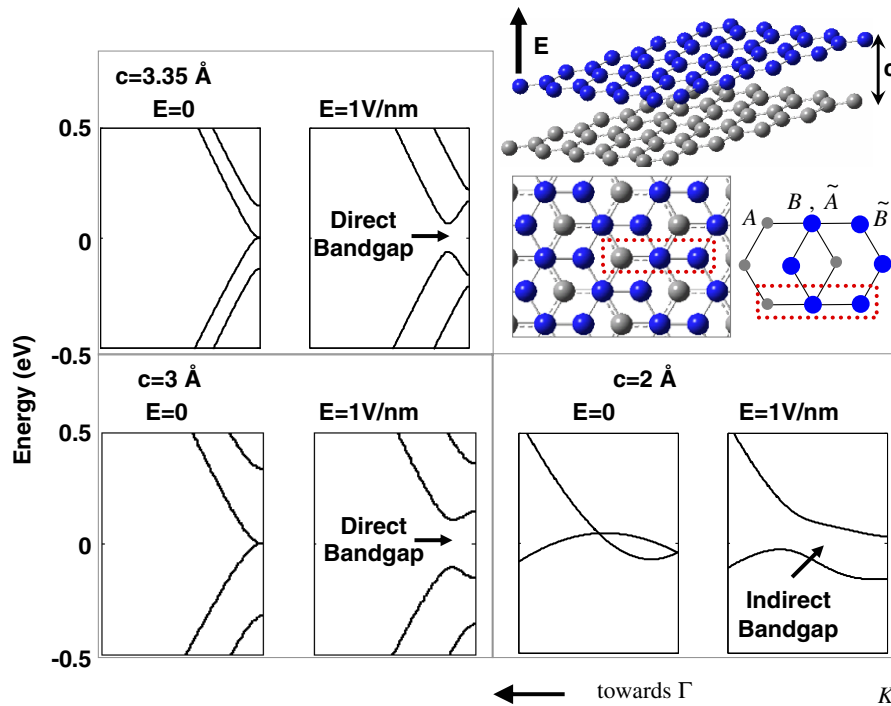
Graphene is a two-dimensional membrane of hexagonally arranged carbon atoms. One obtains zero band gap and linear dispersion around the Dirac point for a monolayer of graphene [1–4]. When two graphene layers are stacked in Bernal ( $\tilde{A}-B$ ) configuration, these monolayer features are lost and the dispersion becomes quadratic [5]. The bilayer configuration is very interesting for various applications, since the band gap can be modulated from zero to a few tens of an electron volt by using an external out-of-plane electric field [5–10] and chemical doping [11].

This electric field breaks the  $A-\tilde{B}$  symmetry in the stacked bilayers and hence lifts the degeneracy. The valence (conduction) band becomes localized on the graphene layer towards positive (negative) gate voltage. The increasing gate voltages in the push/pull configuration lower (raise) the valence (conduction) band, resulting in the band gap opening. The band gap depends on the coupling between the two graphene layers [5, 6]. Therefore, one should be able to tune this band gap by straining the bilayer. This is analogous to piezoresistivity, however the effect is enhanced exponentially due to band gap modification. This could be very useful in sensors and other applications involving strain. Additionally, we find that by straining the bilayer graphene, conduction and valence band dispersions also change.

For electronic structure calculations, we use a semi-empirical extended Hückel theory (EHT) with non-orthogonal

basis set. The detailed model has been described in [10]. The EHT parameters are transferable and have been benchmarked with the graphene band structure using the generalized gradient approximation (GGA) in density function theory. Thus, EHT has many-body exchange–correlation effects at the GGA level. Additionally, this method is computationally very efficient and the non-orthogonality captures the bonding chemistry of various systems very well. It has been applied to armchair graphene nanoribbons [12], large Si systems for electronic structure and quantum transport [13, 14] and single molecule incoherent transport [15, 16] utilizing modest computational resources.

The C–C atomic distance is taken as 1.44 Å within the graphene plane. Out-of-plane equilibrium stacking distance ( $c$ ) is 3.35 Å as shown in figure 1. The gray (light shaded) atoms belong to the lower layer and the blue (dark shaded) atoms represent the upper layer. The unit cell consists of four atoms—two atoms in each layer shown by red (black) dotted line in figure 1. The two gray (light shaded) atoms in the lower layer are referred to as A and B, respectively. The two blue (dark shaded) atoms in the upper layer are referred to as  $\tilde{A}$  and  $\tilde{B}$ , respectively. The electric field is applied in the out-of-plane direction as shown in figure 1. Atomic visualization is done using GaussView [17]. The substrate effects are ignored and in that sense, the graphene bilayer is assumed to be in vacuum.



**Figure 1.** Electronic structure of bilayer graphene.  $E(k)$  diagrams are shown around the Dirac point with and without electric fields. For equilibrium stacking distance  $c = 3.35$  Å, the dispersion is quadratic. With an external electric field, a direct band gap appears. For  $c = 3$  Å, band gap modulation is larger due to increased hopping between the two layers and remains direct. For  $c = 2$  Å, the bilayer becomes metallic with  $E = 0$  and has an indirect band gap for a finite electric field.

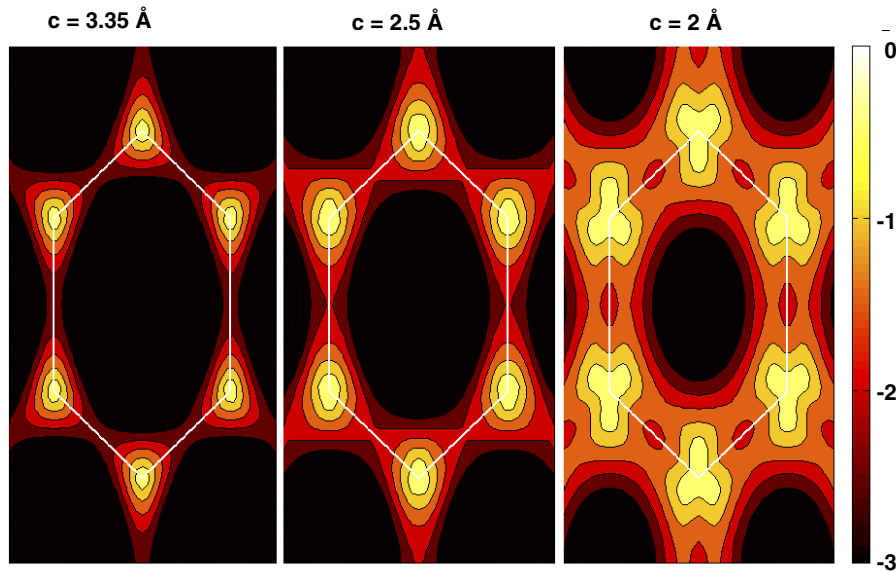
Furthermore, self-consistency is not included in the reported calculations.

The electronic structure calculations for a bilayer graphene with equilibrium stacking distance  $c = 3.35$  Å are shown in figure 1. Without any electric field, the dispersion is quadratic with a zero band gap at the Dirac (K) point. With an electric field of  $1 \text{ V nm}^{-1}$ , a direct band gap opens up due to  $A-\tilde{B}$  symmetry breaking and the conduction (valence) band minimum (maximum) shifts away from the Dirac point. By decreasing  $c$  to  $3$  Å, without an electric field, the band gap is still zero with quadratic dispersion. However, the dispersion changes with an increase in the effective mass and the high lying bands move further away from the Dirac point. With  $E = 1 \text{ V nm}^{-1}$ , again a direct band gap is observed with the same features as the ones for  $c = 3.35$  Å. Apart from this, the band gap modulation is higher for  $c = 3$  Å, although Laplace's potential is smaller for the same electric field due to the reduced spacing. This is due to the increased wavefunction overlap between the two layers, which varies exponentially with distance as compared to Laplace's potential which is linearly dependent on the distance. Further reducing the stacking distance results in a metallic state as shown in figure 1 for  $c = 2$  Å. By applying  $1 \text{ V nm}^{-1}$  electric field, an indirect band gap is created.

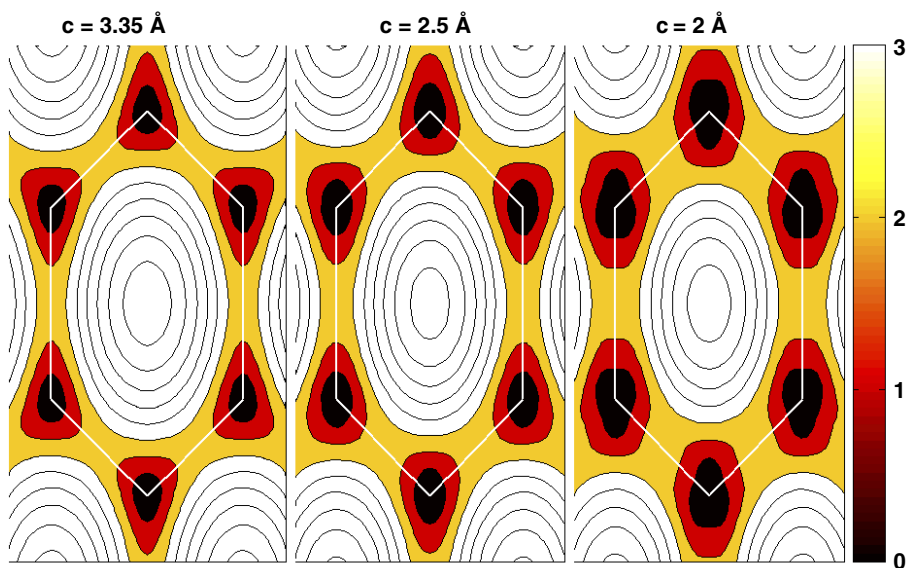
Below about  $2.5$  Å, the distance between atoms in the bottom layer and the next-nearest neighbors in the top layer becomes about  $3.35$  Å, which is the equilibrium stacking distance for bilayer graphene. Therefore, the hopping integral

between  $A-\tilde{B}$  sites becomes comparable to the equilibrium one of the  $\tilde{A}-B$  sites. This results in the reported electronic structure modifications in figure 1 for  $c = 2$  Å. This electronic structure change is also evident in the color plots of the valence band states over the two-dimensional Brillouin zone in figure 2. With decreasing stacking distance from  $c = 3.35$  to  $2.5$  Å in the absence of an electric field, the features become broad indicating an increase in effective mass. Further decreasing  $c$  to  $2$  Å results in directional change of the features, which signifies that the additional bonding happens in different directions than that for  $c = 3.35$  Å. These features are also present in the two-dimensional Brillouin zone of the conduction band states in figure 3. However, it is more evident in the valence band states due to the constructive wavefunction overlap for the bonding nature in contrast to the anti-bonding nature of the conduction band states.

Moreover, we find that the smaller the stacking distance, the higher the band gap modulation by electric fields as shown in figure 4. This is a desirable trait for practical applications. The band gap increases with increasing electric field and then saturates. For the equilibrium  $c = 3.35$  Å, the band gap saturates at about  $0.13$  eV. In the local density approximation [7], the band gap saturates at about  $0.25$  eV. Although the results are different for the two techniques, the general trend after straining the bilayer should remain the same in the two methods. Furthermore, magnetotransport experiment on a bilayer graphene sandwiched between dielectric medium indicate a band gap of about  $0.2$  eV [8].



**Figure 2.** Electronic structure of the valence band of the bilayer graphene. With decreasing stacking distance ( $c$ ), new features appear in the electronic structure due to increased coupling between the two layers. The color bar is in eV.

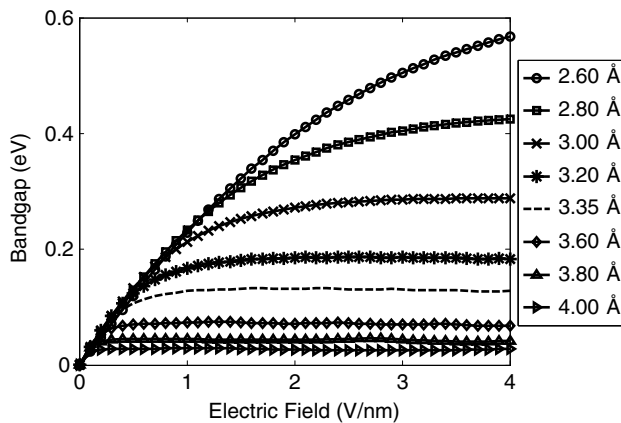


**Figure 3.** Electronic structure of the conduction band of the bilayer graphene with various stacking distances.

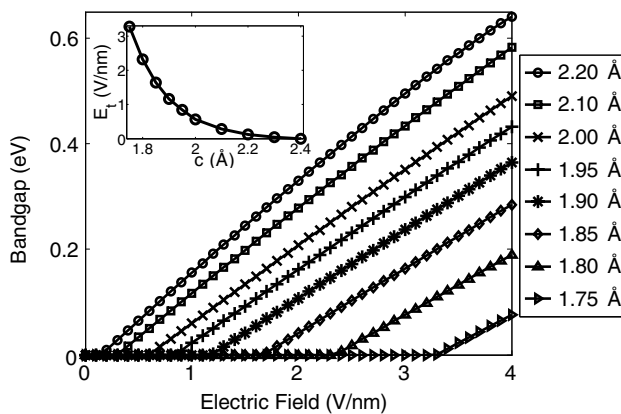
Additionally, angle-resolved photoemission spectroscopy for a bilayer graphene on silicon carbide substrate chemically doped with potassium displays a band gap of about 0.2 eV [11]. Although, these systems are in different chemical and physical environment than ours, the values are still close.

Apart from this, above about 2.5 Å, the trend of field modulation is convex and in the absence of electric field, a zero band gap is observed as shown in figure 4. However, below about 2.5 Å, the systems becomes metallic without electric fields and the trend of field modulation becomes concave, for which a threshold behavior is observed as shown in figure 5. The band gap opening occurs only above a certain threshold

electric field. This threshold value monotonically increases with the decreasing stacking distance as shown in the inset of figure 5. As shown in figure 1, for  $c = 2 \text{ \AA}$ , the valence and conduction bands are overlapping, giving rise to a metallic state. Therefore, a certain electric field needs to be applied to reduce this overlap to zero and then additional electric field opens up the band gap. A band gap of about 0.6 eV can be opened as shown in figures 3 and 4 using a  $4 \text{ V nm}^{-1}$  electric field. Calculations for such a high field are reported to show the band gap saturation and the threshold trends for the strained bilayer. However, these high fields may not be feasible in devices due to the dielectric reliability concerns and physical constraints. High- $K$  dielectrics may be used as an alternative



**Figure 4.** Band gap modulation of strained bilayer with an external electric field. The dashed line is for equilibrium  $c = 3.35$  Å, for which band gap saturates at about 0.13 eV. A convex relation is observed as a function of electric field above  $c \approx 2.5$  Å. By decreasing  $c$ , band gap modulation increases due to increased interlayer hopping.



**Figure 5.** Band gap modulation of strained bilayer with an external electric field. Below about 2.5 Å stacking distance, a concave relation is observed as a function of electric field, where band gap opening occurs only above a threshold electric field ( $E_t$ ). Above  $E_t$ , the band gap linearly increases with external electric field. The inset shows variation of  $E_t$  with  $c$ .

to enhance the field inside the graphene bilayer, while keeping the dielectric within the breakdown regime.

We have analyzed the strain effects on the bilayer graphene using EHT and the corresponding band gap development due to an external electric field. We find that above 2.5 Å stacking distance, the band gap is direct and the band gap follows a convex relation to the electric field. However, below 2.5 Å stacking distance, the band gap becomes indirect and it follows a concave relation.

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